

Diethylene glycol diethyl ether
112-36-7 | DTXSID3025047

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.91 | 1.08 | 0.91 | 1.08 | 0.92 | 1.00 |

Model Results

Predicted value: 6.30e-01 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.97e-01

Confidence level: 5.77e-01

Nearest Neighbors from the Training Set

| | | |
|--|--|---|
| <div>Image not found</div> <div>Isopropyl octadecanoate</div> <div>Measured: 5.20e-01</div> <div>Predicted: 1.13e-05</div> | <div>Image not found</div> <div>Phosmet</div> <div>Measured: 2.30e-02</div> <div>Predicted: 5.53e-07</div> | <div>Image not found</div> <div>Bis(2-chloroethoxy)methane</div> <div>Measured: 2.96</div> <div>Predicted: 1.91e-01</div> |
| <div>Image not found</div> <div>Propham</div> <div>Measured: 3.86</div> <div>Predicted: 1.30e-04</div> | <div>Image not found</div> <div>Propanoic anhydride</div> <div>Measured: 11.0</div> <div>Predicted: 9.92e-01</div> | |